That which is claimed:

1. An isolated polyketide synthase comprising at least fourteen active site α-carbons having the structural coordinates of Table 1.

2. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 164 is alanine or serine.

3. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 303 is alanine, asparagine, glutamine, aspartic acid, or threonine.

4. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 336 is a lysine, alanine, aspartic acid, glutamine, or histidine.

5. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 215 is serine, tyrosine, or tryptophan.

6. The isolated polyketide synthase of claim 1, wherein the polyketide synthase has atomic coordinates as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, or 1D6H.

7. A nucleic acid encoding the synthase of claim 1.

8. A nucleic acid encoding the synthase of claim 2.

9. A nucleic acid encoding the synthase of claim 3.

10. A nucleic acid encoding the synthase of claim 4.

11. A nucleic acid encoding the synthase of claim 5.

12. A method of predicting the activity and/or substrate specificity of a putative polyketide synthase, said method comprising:

comparing the representation of a known polyketide synthase and the representation of a putative polyketide synthase, wherein differences between the two

representations are predictive of polyketide synthase activity and/or substrate specificity.

13. The method of claim 12, wherein the known polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

14. The method of claim 13, wherein the known chalcone synthase has strucutral coordinants as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, or 1CGZ.

15. The method of claim 13, wherein the known pyrone synthase has atomic coordinates as set forth in Table 3.

16. The method of claim 12, wherein the putative synthase is a mutant of a known polyketide synthase.

17. A crystalline form of the polyketide synthase of claim 1.

18. A crystalline form of the polyketide synthase of claim 2.

19. A crystalline form of the polyketide synthase of claim 3.

20. A crystalline form of the polyketide synthase of claim 4.

21. A crystalline form of the polyketide synthase of claim 5.

22. A crystalline chalcone synthase, stilbene synthase, or pyrone synthase..

23. A crystalline complex comprising chalcone synthase and a chalcone synthase substrate.

24. The crystalline complex of claim 23, wherein the chalcone synthase is native chalcone synthase.

25. The crystalline complex of claim 23, wherein the chalcone synthase is a non-native chalcone synthase.

26. The crystalline complex of claim 23, wherein the chalcone synthase substrate is selected from the group consisting of chalcone, naringenin, resveratrol, cerulenin, acyl-CoA, malonyl-CoA, and hexanoyl-CoA.

27. The crystalline complex of claim 23, wherein the complex has atomic coordinates as set forth in PDB Accession Nos: 1BQ6, 1CML, 1CHW, 1CGK or 1CGZ.

28. A method of identifying a potential substrate of a polyketide synthase, said method comprising:

(a) defining the active site of said polyketide synthase based on a plurality of atomic coordinates of said polyketide synthase,

(b) identifying a potential substrate that fits the active site of (a) with the polyketide synthase, and

(c) contacting the polyketide synthase with the potential substrate and determining its activity thereon.

29. The method of claim 28, wherein the polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

30. The method of claim 28, wherein the polyketide synthase is a mutant of a known polyketide synthase.

31. The method of claim 30, wherein the known polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

32. The method of claim 28, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, or portions thereof.

33. A method of identifying a potential inhibitor of a polyketide synthase, said method comprising:

(a) defining the active site of said polyketide synthase based on a plurality of atomic coordinates of said polyketide synthase,

(b) contacting a potential compound that fits the active site of (a) with the polyketide synthase in the presence of a substrate, and

(c) determining the ability of said compound to inhibit the activity of said polyketide synthase on said substrate.

34. The method of claim 33, wherein the polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

35. The method of claim 33, wherein the polyketide synthase is a mutant of a known polyketide synthase.

36. The method of claim 35, wherein the mutant polyketide synthase is a mutant of chalcone synthase, stilbene synthase, and pyrone synthase.

37. The method of claim 33, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, or portions thereof.

38. A computer program on a computer readable medium, said computer program comprising instructions to cause a computer to:

define a polyketide synthase or fragment thereof based on a plurality of atomic coordinates of the polyketide synthase.

39. The computer program of claim 38, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, Table 3, or portions thereof.